A general expression for the excitation cross section of polarized atoms by polarized electrons

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Abstract. The general expression for excitation cross section of polarized atoms by polarized electrons is derived by using the methods of the theory of an atom adapted for polarization. The special cases of the general expression for the description of the angular distribution and alignment of excited atoms in the case of polarized and non-polarized atoms as well as the magnetic dichroism of the total ionization cross section of polarized atoms are obtained. The cross sections and alignment parameters for the excitation of the autoionizing states $2p^5 3s^2\ ^2P_{3/2}$ for Na and $3p^5 4s^2\ ^2P_{3/2}$ for K are calculated in distorted wave with exchange approximation.

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1. Introduction

Polarized atoms and ions presents in plasma where directed flows of charged particles take place. The directed movement of these particles is very important in laboratory and astrophysical plasmas resulting in the distortion of Maxwellian distribution of electrons [1]. The non-equilibrium population of magnetic sub-levels or the ordering of angular momentum of atomic particles that is called a self-alignment is causes the polarization of the emitted electromagnetic fluorescence radiation that could be used for the fusion plasma diagnostics [2]. Recently, the methods of the theory of an atom were applied for the derivation of the general expressions describing the interaction of polarized photons and electrons with polarized atoms and ions [3-9]. The probability (cross section) of the interaction was expressed as multiple expansion over the multipoles (irreducible tensors) of the state of all particles taking part in the process both in initial and final states. The applied approach was an alternative to the density matrix method [10] where the density matrix elements were expressed via multipoles or statistical tensors. The density matrix formalism was used for the study of some special cases of the polarization of the particles presented in the excitation process. These expressions were applied for the calculations of the alignment of autoionizing states of alkaline atoms excited by electrons [11, 12, 13], positrons [11] or other charged particles [12] The expressions for the description of the polarization and angular distribution of the radiation from unpolarized atoms excited by polarized electrons were derived by Bartschat *et al* [14] in a general case. These expressions were applied for the calculation of the electron impact excitation of the 4 ^{1}P$_1$ state of calcium [15, 16].

The main task of the present work was the derivation of a general expression describing the polarization state of all particles taking part in the excitation of polarized atoms by polarized electrons with the help of the method based on the theory of an atom [3]. The next section of the present work is devoted to obtaining of the general expression. Its special cases as well the calculations of total cross section and alignment parameters are presented in Section 3. The inequality

$$\text{fine structure splitting} \gg \text{line width} \gg \text{hyperfine structure splitting}$$

is also assumed. The modifications enabling to take into account hyperfine structure splitting can be easily made [3, 5].

2. General expression

For the excitation of an atom A in the state $\alpha_0 J_0 M_0$ by an electron e^- moving with the momentum $\mathbf{p}_1$ and spin projection m_1

$$A(\alpha_0 J_0 M_0) + e^-(\mathbf{p}_1 m_1) \to A(\alpha_1 J_1 M_1) + e^-(\mathbf{p}_2 m_2), \tag{1}$$

the cross section can be written in atomic system of units as follows:

$$\frac{d\sigma(\alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \to \alpha_1 J_1 M_1 \mathbf{p}_2 m_2)}{d\Omega_2} = \frac{p_2}{(2\pi)^2 p_1} \langle \alpha_1 J_1 M_1 \mathbf{p}_2 m_2 | V | \alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \rangle$$

$$\times \langle \alpha_1 J_1 M_1 \mathbf{p}_2 m_2 | V | \alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \rangle^* \delta(E_0 - E_1). \quad (2)$$

Here V is the operator of the electrostatic interaction between projectile and atomic electrons, E_0 and E_1 are the energies of the system atom+electron in the initial and final states, p_i is the absolute value of the momentum,$p_i = \sqrt{2\varepsilon_i}$, ε_i is the energy of the projectile electron in the initial ($i = 1$) and final ($i = 2$) states, $\alpha_2 J_2 M_2$ and $\mathbf{p}_2 m_2$ describe the states of the excited atom and scattered electron, respectively.

The wave function of the projectile and scattered electrons can be expressed via expansion over Spherical harmonics

$$|\mathbf{p}m\rangle = 4\pi \sum_{\lambda\mu} R_\lambda(r) Y_{\lambda\mu}(\hat{r}) Y^*_{\lambda\mu}(\hat{p}) \xi_m(\sigma)$$

$$= \sum_{\lambda\mu} \sqrt{4\pi(2\lambda+1)} R_\lambda(r) C^{(\lambda)}_\mu(\hat{r}) Y^*_{\lambda\mu}(\hat{p}) \xi_m(\sigma). \quad (3)$$

Here $\xi_m(\sigma)$ is the spin orbital of an electron, $C^{(\lambda)}_\mu(\hat{r})$ is the operator of the spherical function [17], where $\hat{r}$ denotes the polar and azimutal angles of the spherical coordinate system,

$$R^*_\lambda(r) = \mathrm{i}^\lambda \exp[\mathrm{i}(\sigma_\lambda(p) + \delta_\lambda)] r^{-1} P(\varepsilon\lambda|r) \quad (4)$$

is the radial orbital of the electron in a continuum state normalized to $\delta(\varepsilon - \varepsilon')$. For the electron moving in the field of an ion, the asymptotic of the Hartree orbital $P(\varepsilon\lambda|r)$ is

$$P(\varepsilon\lambda|r \to \infty) \sim (\pi p)^{-1/2} \sin(pr - \lambda\pi/2 + Z_{ef} \ln(2pr)/p + \sigma_\lambda(p) + \delta_\lambda) \quad (5)$$

with Coulomb phase

$$\sigma_\lambda(p) = arg\, \Gamma(\lambda + 1 - \mathrm{i}(Z_{ef} - 1)/p) \quad (6)$$

and effective nuclear charge $Z_{ef} = Z - N + 1$. Here Z is the nuclear charge, N is the number of electrons. In (5), δ_λ is the phase arising due to the deviation of the self consistent field from Coulomb one. In the case of neutral atom, the asymptotic expression of Hartree orbital obtains the following expression:

$$P(\varepsilon\lambda|r \to \infty) \sim (\pi p)^{-1/2} \sin(pr - \lambda\pi/2 + \delta_\lambda). \quad (7)$$

The substitution of (3) into (2) leads to the following expression for one transition matrix element:

$$\langle \alpha_1 J_1 M_1 \mathbf{p}_1 m_1 | H | \alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \rangle = \sum_{\substack{\tilde{M}_0, \tilde{M}_1, \tilde{m}_1, \tilde{m}_2, \\ \lambda_1, \mu_1, \lambda_2, \mu_2}} [(2\lambda_1+1)(2\lambda_2+1)]^{1/2}$$

$$\times \langle \alpha_1 J_1 \tilde{M}_1 \varepsilon_1 \lambda_1 \mu_2 \tilde{m}_1 | H | \alpha_0 J_0 \tilde{M}_0 \varepsilon_1 \lambda_1 \mu_1 \tilde{m}_1 \rangle D^{J_0}_{\tilde{M}_0 M_0}(\hat{J}_0)\; D^{*J_1}_{\tilde{M}_1 M_1}(\hat{J}_1)\; D^{\lambda_1}_{\mu_1 0}(\hat{p}_1)$$

$$\times D^{*\lambda_2}_{\mu_2 0}(\hat{p}_2)\; D^{s}_{\tilde{m}_1 m_1}(\hat{s})\; D^{*s}_{\tilde{m}_2 m_2}(\hat{s}). \tag{8}$$

Here the possibility of the registration of the orientation of angular momentum of all particles with respect to different quantization axes is taken into account. For the evaluation of the matrix element, the wave functions of all particles taking part in the process were transformed to the same system of coordinates by using the transformation procedure

$$|j\tilde{m}\rangle = \sum_m D^{j}_{m\tilde{m}}(\alpha,\beta,\gamma)|jm\rangle. \tag{9}$$

Here $D^{j}_{m\tilde{m}}(\alpha,\beta,\gamma)$ is the Wigner rotation matrix.

The integration over orbital and summation over spin variables was performed with the help of the graphical technique of the angular momentum [17, 18]. The angular momentum diagrams used for the derivation of the general expression of the excitation cross section of polarized atoms by polarized electrons are represented in figures 1 and 2. The angular part of the matrix element (8) is represented in diagram E_1 (see figure 1). Here the rectangle with (kk) indicates the orbital and spin parts of the electrostatic interaction operator which orbital part is defined as follows:

$$V = \sum_k \frac{r^k_<}{r^{k+1}_>}(C^{(k)}_1 C^{(k)}_2).$$

Here and 1 and 2 show the atomic and projectile electrons, respectively. Other rectangles in diagram E_1 represent the orbital and spin parts of the configuration and other quantum numbers. The circles with D inside are Wigner rotation matrices. The electron was excited from the shell which orbital quantum number is l_0 to the shell which orbital quantum number is l_1, and $s = 1/2$.

To extract the reduced matrix element from diagram E_1, one needs to cut of the Wigner rotation matrices from the open lines of each angular momentum (circles with D) and to choose the order of the coupling of open lines. Let us choose the following order of coupling: $J_0, \lambda_1 s(j_1)J$ and $J_1, \lambda_2 s(j_2)J$. Then the procedure of the extraction of the reduced matrix element may be written by using the diagrams from figure 1

$$\mathrm{E}_1 = \sum_{j_1,j_2,J} (2J+1)\; \mathrm{E}_2\; \mathrm{E}'_3, \tag{10}$$

where E_2 is the angular part of the diagram of reduced matrix element $\langle \alpha_1 J_1, \varepsilon_2 \lambda_2(j_2)J||H||\alpha_0 J_0, \varepsilon_1\lambda_1(j_1)J\rangle$ and E'_3 is the generalized Clebsch-Gordan coefficient [17] represented by the left side of diagram E_3. The right side of diagram E_3 comes from the angular part of the complex conjugate matrix element from (2).

For further simplification of the part describing the space rotation dependence, the following expansion can be used:

$$D^{J}_{\tilde{M}M}(\hat{J})\; D^{*J'}_{\tilde{M}'M}(\hat{J}) = \sum_{K,N} T^{*K}_N(\hat{J}) \begin{bmatrix} J' & K & J \\ \tilde{M}' & N & \tilde{M} \end{bmatrix}. \tag{11}$$

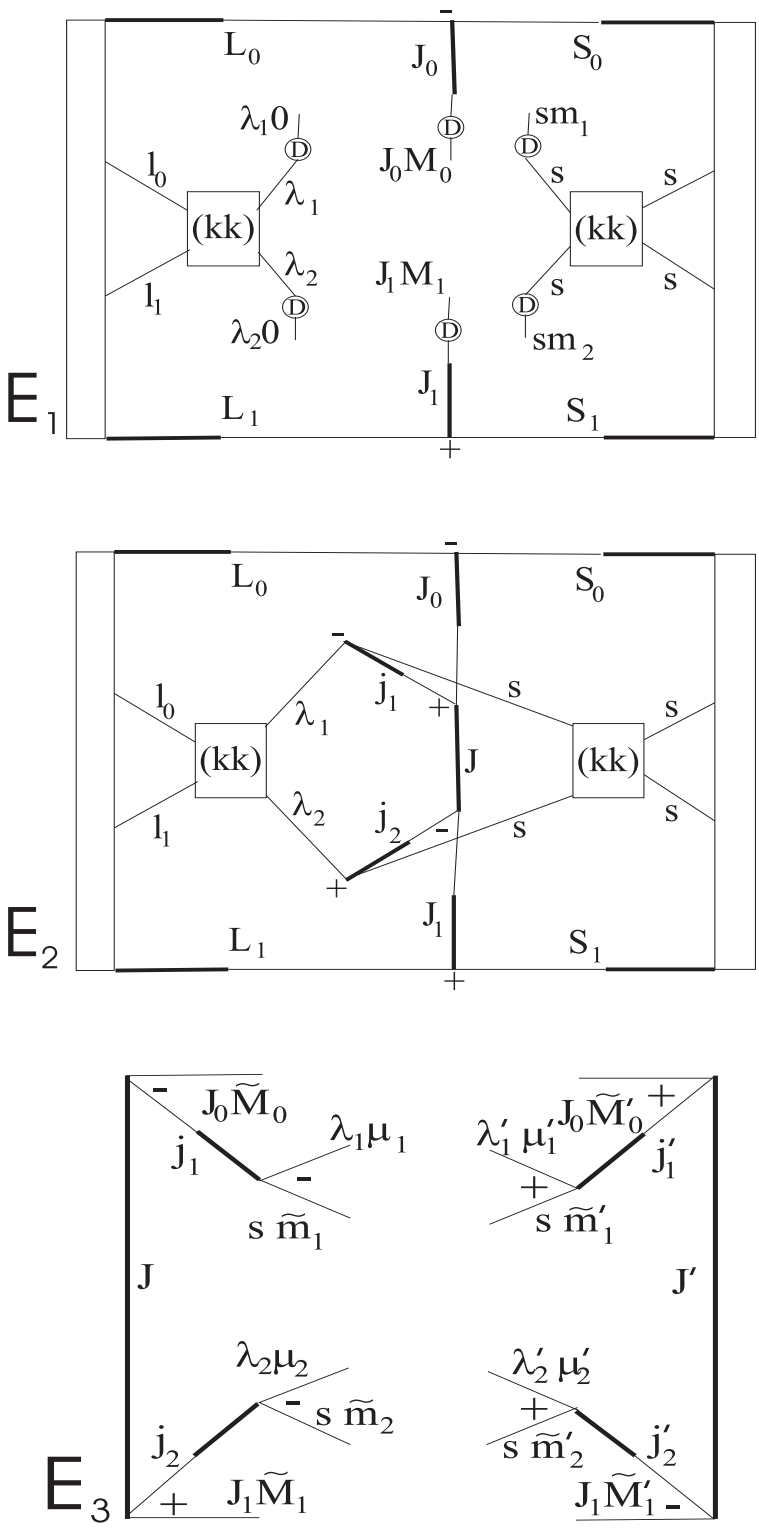

Figure 1 The angular momentum diagrams used for the derivation of the general expression of the excitation cross section of polarized atoms by polarized electrons.

In(11), the angle brackets with angular momenta inside show the Clebsch-Gordan coefficient [17], and the tensor is defined [8] as

$$T_N^{*K}(\hat{J}) = (-1)^{J'-M}\left[\frac{4\pi}{2J+1}\right]^{1/2}\left[\begin{array}{ccc} J & J' & K \\ M & -M & 0 \end{array}\right] Y_{KN}^{*}(\theta,\phi). \qquad (12)$$

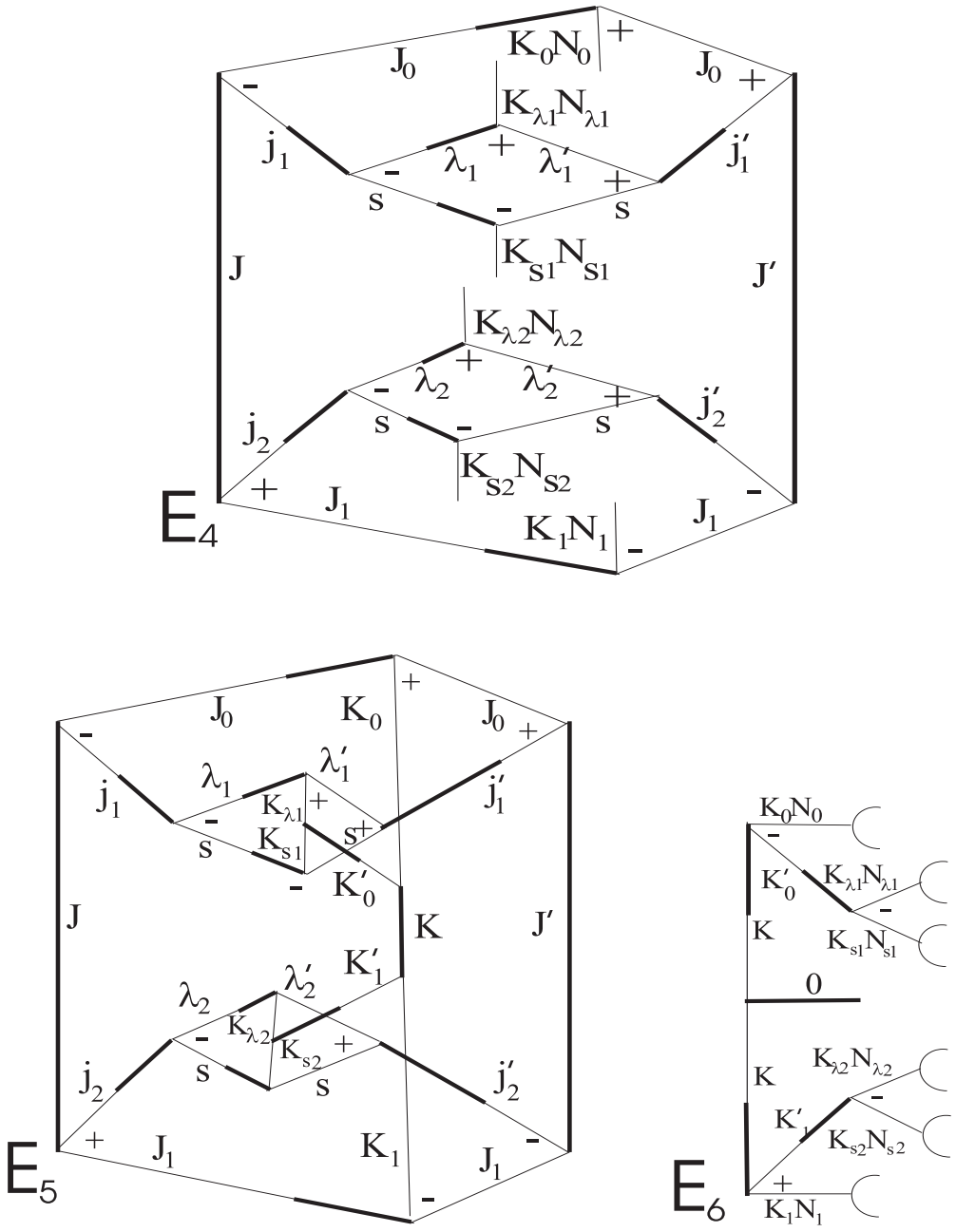

Figure 2 The angular momentum diagrams used for the derivation of the general expression of the excitation cross section of polarized atoms by polarized electrons.

Six Clebsch-Gordan coefficients obtained by applying (12) for all angular momenta $\lambda_1, \lambda_2, J_0, J_1$ and two spins s of free electrons are used to perform the summation over the projections $\tilde{M}_0, \tilde{M}'_0, \tilde{M}_1, \tilde{M}'_1,\ \tilde{\mu}_1, \tilde{\mu}'_1, \tilde{\mu}_1, \tilde{\mu}'_1, \tilde{m}_1, \tilde{m}'_1, \tilde{m}_2, \tilde{m}'_2$ of the matrix element in (8) and its complex conjugate. This summation was performed graphically, and the result is represented by diagram E_4 (see figure 2) that looks rather complicated. But further simplifications of E_4 are still possible. The closing of the open lines from diagram E_4 produces diagram E_5 invariant under space rotation and diagram E_6 describing rotation

properties of the cross section (2). The bow at the end of each open line stands for the tensor (12) [5] in the case of J_0, J_1, spin s and spherical function for λ_1, and λ_2. Four 9j-coefficients [17] can be obtained from diagram E_5 by cutting it trough the lines $(J, K, J'), (j_1, K'_0, j'_1)$ and (j_2, K'_1, j'_2).

The final expression for the cross section (2) obtained by using diagrams E_2, E_5 and E_6 is as follows:

$$\frac{d\sigma(\alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \to \alpha_1 J_1 M_1 \mathbf{p}_2 m_2)}{d\Omega}$$

$$= 4\pi C \sum_{\substack{K, K_0, K'_0, K_{\lambda 1}, K_{s1}, K_1 \\ K'_1, K_{\lambda 2}, K_{s2}}} \mathcal{B}^{\rm ex}(K_0, K'_0, K_1, K'_1, K_{\lambda 1}, K_{s1}, K_{\lambda 2}, K_{s2}, K)$$

$$\times \sum_{\substack{N_0, N'_0, N_{\lambda 1}, N_{s1}, N_1 \\ N'_1, N_{\lambda 2}, N_{s2}, N}} \begin{bmatrix} K_{\lambda 1} & K_{s1} & K'_0 \\ N_{\lambda 1} & N_{s1} & N'_0 \end{bmatrix} \begin{bmatrix} K_0 & K'_0 & K \\ N_0 & N'_0 & N \end{bmatrix} \begin{bmatrix} K_1 & K'_1 & K \\ N_1 & N'_1 & N \end{bmatrix}$$

$$\times \begin{bmatrix} K_{\lambda 2} & K_{s2} & K'_1 \\ N_{\lambda 2} & N_{s2} & N'_1 \end{bmatrix} Y^*_{K_{\lambda 1} N_{\lambda 1}}(\hat{p}_1)\, Y_{K_{\lambda 2} N_{\lambda 2}}(\hat{p}_2)\, T^{*K_0}_{N_0}(J_0, J_0, M_0|\hat{J}_0)\, T^{K_1}_{N_1}(J_1, J_1, M_1|\hat{J}_1)$$

$$\times T^{*K_{s1}}_{N_{s1}}(s, s, m_1|\hat{s})\, T^{K_{s2}}_{N_{s2}}(s, s, m_2|\hat{s}), \tag{13}$$

$$\mathcal{B}^{\rm ex}(K_0, K'_0, K_1, K'_1, K_{\lambda 1}, K_{s1}, K_{\lambda 2}, K_{s2}, K)$$

$$= \sum_{\lambda_1, \lambda'_1, \lambda_2, \lambda'_2, j_1, j'_1, j_2, j'_2, J, J'} (2J+1)(2J'+1)(2s+1)(-1)^{\lambda'_1 + \lambda'_2}$$

$$\times \langle \alpha_1 J_1, \varepsilon_2 \lambda_2(j_2) J || H || \alpha_0 J_0, \varepsilon_1 \lambda_1(j_1) J \rangle \langle \alpha_1 J_1, \varepsilon_2 \lambda'_2(j'_2) J' || H || \alpha_0 J_0, \varepsilon_1 \lambda'_1(j'_1) J' \rangle^*$$

$$\times [(2\lambda_1+1)(2\lambda'_1+1)(2\lambda_2+1)(2\lambda'_2+1)(2j_1+1)(2j'_1+1)(2j_2+1)(2j'_2+1)$$

$$\times (2J_0+1)(2J_1+1)(2K'_0+1)(2K'_1+1)]^{1/2} \begin{bmatrix} \lambda_1 & \lambda'_1 & K_{\lambda 1} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \lambda_2 & \lambda'_2 & K_{\lambda 2} \\ 0 & 0 & 0 \end{bmatrix}$$

$$\times \begin{Bmatrix} J_0 & K_0 & J_0 \\ j'_1 & K'_0 & j_1 \\ J' & K & J \end{Bmatrix} \begin{Bmatrix} \lambda'_1 & K_{\lambda 1} & \lambda_1 \\ s & K_{s1} & s \\ j'_1 & K'_0 & j_1 \end{Bmatrix} \begin{Bmatrix} \lambda'_2 & K_{\lambda 2} & \lambda_2 \\ s & K_{s2} & s \\ j'_2 & K'_1 & j_2 \end{Bmatrix} \begin{Bmatrix} J_1 & K_1 & J_1 \\ j'_2 & K'_1 & j_2 \\ J' & K & J \end{Bmatrix}. \tag{14}$$

Taking into account the equation (3) and asymptotics (5) and (6), the constant in (2) is $C = 4/p_1^2$.

The expression (13) represents the most general case of the cross section describing the excitation of polarized atoms by polarized electrons and enabling one to obtain information on the angular distributions and spin polarization of scattered electron and the alignment of excited atom in non relativistic approximation.

3. Special cases

3.1. Total cross section for the excitation of unpolarized atoms

In the case when the polarization state of excited atoms and scattered electrons are not registered, the total cross section describing the excitation of unpolarized atoms by unpolarized electrons can be obtained from the general expression (13) by summation

over the magnetic components of the particles in the final state and averaging over them in the initial state as well as integration over the angles of scattered electron. The expression under consideration was obtained by applying the formulas [3]

$$\sum_M T_N^K(J,J,M|\hat{J}) = \delta(K,0)\delta(N,0), \tag{15}$$

$$\int_0^\pi \int_0^{2\pi} \sin\theta d\theta d\phi Y_{KN}(\theta,\phi) = \sqrt{4\pi}\delta(K,0)\delta(N,0) \tag{16}$$

and is as follows:

$$\sigma(\alpha_0 J_0 \to \alpha_1 J_1) = \frac{1}{2(2J_0+1)} \int d\Omega \sum_{M_0,m_1,M_1,m_2} \frac{d\sigma(\alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \to \alpha_1 J_1 M_1 \mathbf{p}_2 m_2)}{d\Omega}$$

$$= \frac{4\pi}{(2J_0+1)\varepsilon_1} \mathcal{B}^{\rm ex}(0,0,0,0,0,0,0,0,0). \tag{17}$$

Here

$$\mathcal{B}^{\rm ex}(0,0,0,0,0,0,0,0,0)$$

$$= \sum_{\lambda_1,j_1,\lambda_2,j_2,J} (2J+1)|\langle \alpha_1 J_1, \varepsilon_2\lambda_2(j_2)J||H||\alpha_0 J_0, \varepsilon_1\lambda_1(j_1)J\rangle|^2. \tag{18}$$

3.2. The angular distribution of scattered electrons following the excitation of unpolarized atoms

The excitation of unpolarized atoms by unpolarized electrons is usual and often occurred process in plasmas. To obtain the expression of the differential cross section suitable for the description of the angular distribution of scattered electrons one needs to performer the summation of the general expression (13) over the magnetic components of the particles in the final state and averaging over them in the initial state. The application of the expression (15) and the choice of the laboratory quantization axes along the direction of the projectile electron, that means $Y_{KN}(0,0) = [(2K+1)/4\pi]^{1/2}\delta(N,0)$, leads to the expression

$$\frac{d\sigma(\alpha_0 J_0 \to \alpha_1 J_1 \mathbf{p}_2)}{d\Omega} = \frac{1}{2(2J_0+1)} \sum_{M_0,m_1,M_1,m_2} \frac{d\sigma(\alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \to \alpha_1 J_1 M_1 \mathbf{p}_2 m_2)}{d\Omega}$$

$$= \frac{\sigma(\alpha_0 J_0 \to \alpha_1 J_1)}{4\pi} \left[1 + \sum_{K>0} \beta_K P_K(\cos\theta)\right]. \tag{19}$$

Here the asymmetry parameters of the angular distribution of the scattered electrons are defined as follows:

$$\beta_K = \frac{(2K+1)\mathcal{B}^{\rm ex}(0,K,0,K,K,0,K,0,K)}{\mathcal{B}^{\rm ex}(0,0,0,0,0,0,0,0,0)}. \tag{20}$$

In (19), the summation parameter K can acquire the values $\max\{|\lambda_1-\lambda_1'|,|\lambda_2-\lambda_2'|\} \le K \le \min\{\lambda_1+\lambda_1',\lambda_2+\lambda_2'\}$ for each set of the partial wave momenta which can be very large depending on the energy of the projectile electron. Several partial waves are enough only for the energies close to the excitation threshold.

3.3. The angular distribution of scattered electrons following the excitation of polarized atoms

In the case of the atoms prepared in polarized state, the expression for the differential cross section describing the angular distribution of the scattered electrons can be also obtained by the summation over the magnetic components of the particles in the final state and averaging over the states of the spin in the initial state in the general expression (13). In the case of the choice of the laboratory quantization axes along the direction of the projectile electron, the expression for the cross section is as follows:

$$\frac{d\sigma(\alpha_0 J_0 M_0 \to \alpha_1 J_1 \mathbf{p}_2)}{d\Omega} = \frac{1}{2}\sum_{m_1,M_1,m_2}\frac{d\sigma(\alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \to \alpha_1 J_1 M_1 \mathbf{p}_2 m_2)}{d\Omega}$$

$$= \frac{C\sqrt{4\pi}}{2}\sum_{K_{\lambda_1},K_0,K_{\lambda_2},N_0}[2K_{\lambda_1}+1]^{1/2}\mathcal{B}^{\rm ex}(K_0,K_{\lambda_1},0,K_{\lambda 2},K_{\lambda 1},0,K_{\lambda 2},0,K_{\lambda 2})$$

$$\times\begin{bmatrix} K_0 & K_{\lambda_1} & K_{\lambda_2} \\ N_0 & 0 & N_0 \end{bmatrix} Y_{K_{\lambda_2}N_0}(\hat{p}_2)\left[\frac{4\pi}{2J_0+1}\right]^{1/2}(-1)^{J_0-M_0}\begin{bmatrix} J_0 & J_0 & K_0 \\ M_0 & -M_0 & 0 \end{bmatrix}$$

$$\times Y^*_{K_0N_0}(\hat{J}_0). \qquad (21)$$

This expression becomes more simple in the case of special geometry of the experiment. If the atom is polarized along the direction of the projectile electron, then $N_0 = 0$, $M_0 = J_0$, $Y^*_{K_0N_0}(0,0) = \sqrt{(2K_0+1)/4\pi}\delta(N_0,0)$, $Y_{K_{\lambda_2}0}(\hat{p}_2) = \sqrt{(2K_{\lambda_2}+1)/4\pi}P_{K_{\lambda_2}}(\cos\theta)$, and the angle θ is measured from the direction of the projectile electron. Then the expression (21) transforms into the following expression:

$$\frac{d\sigma(\alpha_0 J_0 M_0 = J_0 \to \alpha_1 J_1 \mathbf{p}_2)}{d\Omega} = \frac{\sigma(\alpha_0 J_0 \to \alpha_1 J_1)}{4\pi}\left[1+\sum_{K_{\lambda_2}>0}B_{K_{\lambda_2}}P_{K_{\lambda_2}}(\cos\theta)\right]. \qquad (22)$$

Here

$$B_{K_{\lambda_2}} = \mathcal{B}^{\rm ex}(0,0,0,0,0,0,0,0,0)^{-1}\sum_{K_0,K_{\lambda_1}}\mathcal{B}^{\rm ex}(K_0,K_{\lambda_1},0,K_{\lambda 2},K_{\lambda 1},0,K_{\lambda 2},0,K_{\lambda 2})$$

$$\times[(2J_0+1)(2K_0+1)(2K_{\lambda_1}+1)(2K_{\lambda_2}+1)]^{1/2}\begin{bmatrix} K_0 & K_{\lambda_1} & K_{\lambda_2} \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} J_0 & J_0 & K_0 \\ J_0 & -J_0 & 0 \end{bmatrix} \qquad (23)$$

is one from the set of the asymmetry parameters of the angular distribution of the scattered electrons. The difference of the expression (23) and that with opposite directions of $\mathbf{J}_0$ is equal to the magnetic dichroism in the electron-impact excitation cross section of polarized atoms describing the angular distribution of the scattered electrons.

3.4. Magnetic dichroism in the total electron-impact excitation cross section of polarized atoms

The total cross section of the excitation of polarized atoms by unpolarized electrons can be easily obtained by integration of (21) over the angles of the scattered electrons.

Then $K_{\lambda_2} = N_{\lambda_2} = 0$, $K_0 = K_{\lambda_2}$. This cross section depends on the direction of the polarization of atoms and is as follows:

$$\sigma(\alpha_0 J_0 M_0 \mathbf{p}_1 \to \alpha_1 J_1) = 2\pi\, C \sum_{K_0,N_0} \frac{1}{[(2J_0+1)(2K_0+1)]^{1/2}} (-1)^{K_0+J_0-M_0} \begin{bmatrix} J_0 & J_0 & K_0 \\ M_0 & M_0 & 0 \end{bmatrix}$$

$$\times\, \mathcal{B}^{\rm ex}(K_0, K_0, 0, 0, K_0, 0, 0, 0, 0) Y_{K_0 N_0}(\hat{p}_1) Y^*_{K_0 N_0}(\hat{J}_0). \tag{24}$$

In the case of the choice of the quantization axis z along the direction of the projectile electron, the expression (24) becomes more simple:

$$\sigma(\alpha_0 J_0 M_0 \to \alpha_1 J_1) = 2\pi\, C \sum_{K_0} (-1)^{K_0+J_0-M_0} \left[\frac{2K_0+1}{2J_0+1}\right]^{1/2} \begin{bmatrix} J_0 & J_0 & K_0 \\ J_0 & -J_0 & 0 \end{bmatrix}$$

$$\times\, \mathcal{B}^{\rm ex}(K_0, K_0, 0, 0, K_0, 0, 0, 0, 0) P_{K_0}(\cos\theta), \tag{25}$$

where the angle θ of the orientation of the total angular momentum J_0 of an atom is measured from the direction of the projectile electron.

The degree of magnetic dichroism can be defined by the parameter a which equals to

$$a = \frac{\sigma(\alpha_0 J_0 M_0 \to \alpha_1 J_1) - \sigma(\alpha_0 J_0 - M_0 \to \alpha_1 J_1)}{\sigma(\alpha_0 J_0 M_0 \to \alpha_1 J_1) + \sigma(\alpha_0 J_0 - M_0 \to \alpha_1 J_1)}$$

$$= \frac{\sum_{K_0=odd} B(K_0) P_{K_0}(\cos\theta)}{\sum_{K_0=even} B(K_0) P_{K_0}(\cos\theta)}, \tag{26}$$

where

$$B(K) = (-1)^K \sqrt{2K+1} \begin{bmatrix} J_0 & J_0 & K \\ J_0 & -J_0 & 0 \end{bmatrix} \mathcal{B}^{\rm ex}(K, K, 0, 0, K, 0, 0, 0, 0). \tag{27}$$

Here the values of the summation parameter are $K_0 \le 2J_0$. If the total angular momentum of an atom J_0 is directed along and opposite directions of the projectile electron, then $M_0 = J_0$, $P_{K_0}(0) = 1$, and the parameter of the diamagnetic dichroism is as follows:

$$a = \frac{\sum_{K_0=odd} B(K_0)}{\sum_{K_0=even} B(K_0)}. \tag{28}$$

For small values of the total angular momentum of an atom, the expression of the magnetic dichroism is presented as an example. In the case of $J_0 = 1/2$, it is as follows:

$$a = -\sqrt{3} \frac{\mathcal{B}^{\rm ex}(1, 1, 0, 0, 1, 0, 0, 0, 0)}{\mathcal{B}^{\rm ex}(0, 0, 0, 0, 0, 0, 0, 0, 0)}. \tag{29}$$

For $J_0 = 1$, the magnetic dichroism is defined by the expression:

$$a = \frac{-(3/\sqrt{2})\, \mathcal{B}^{\rm ex}(1, 1, 0, 0, 1, 0, 0, 0, 0)}{\mathcal{B}^{\rm ex}(0, 0, 0, 0, 0, 0, 0, 0, 0) + \sqrt{5/2}\, \mathcal{B}^{\rm ex}(2, 2, 0, 0, 2, 0, 0, 0, 0)}. \tag{30}$$

3.5. The alignment of unpolarized atoms excited by electron-impact

Usually the alignment of the excited atom effects the characteristics of the second step processes [7, 8]. Therefore the special expression should be used in this case. It can be obtained with the help of the method presented by Kupliauskienė [3, 7] for (13) and is as follows:

$$\frac{d\sigma_{K_1N_1}(\alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \to \alpha_1 J_1 \mathbf{p}_2 m_2)}{d\Omega}$$
$$= 4\pi C[2K_1+1]^{1/2} \sum_{\substack{K, K_0, K_0', K_{\lambda 1}, K_{s1} \\ K_1', K_{\lambda 2}, K_{s2}}} \mathcal{B}^{\rm ex}(K_0, K_0', K_1, K_1', K_{\lambda 1}, K_{s1}, K_{\lambda 2}, K_{s2}, K)$$
$$\times \sum_{\substack{N_0, N_0', N_{\lambda 1}, N_{s1} \\ N_1', N_{\lambda 2}, N_{s2}, N}} \left[\begin{array}{ccc} K_{\lambda 1} & K_{s1} & K_0' \\ N_{\lambda 1} & N_{s1} & N_0' \end{array} \right] \left[\begin{array}{ccc} K_0 & K_0' & K \\ N_0 & N_0' & N \end{array} \right] \left[\begin{array}{ccc} K_1 & K_1' & K \\ N_1 & N_1' & N \end{array} \right]$$
$$\times \left[\begin{array}{ccc} K_{\lambda 2} & K_{s2} & K_1' \\ N_{\lambda 2} & N_{s2} & N_1' \end{array} \right] Y^*_{K_{\lambda 1}N_{\lambda 1}}(\hat{p}_1)\, Y_{K_{\lambda 2}N_{\lambda 2}}(\hat{p}_2)\, T^{*K_0}_{N_0}(J_0, J_0, M_0|\hat{J}_0)\, T^{*K_{s1}}_{N_{s1}}(s, s, m_0|\hat{s})$$
$$\times T^{K_{s2}}_{N_{s2}}(s, s, m_1|\hat{s}). \qquad (31)$$

The cross section describing the alignment of excited atoms can be obtained by the integration over the angles of scattered electrons, summation over the magnetic components of the spin of scattered electrons and averaging over the states of atoms and electrons in the initial state of the expressions (31). Its expression is as follows:

$$\sigma_{K_1N_1}(\alpha_0 J_0 \mathbf{p}_1 \to \alpha_1 J_1) = \sum_{K_1} \frac{1}{2(2J_0+1)} \int d\Omega \sum_{M_0, m_1, m_2} \frac{d\sigma_{K_1N_1}(\alpha_0 J_0 M_0 \mathbf{p}_1 m_1 \to \alpha_1 J_1 M_1 \mathbf{p}_2 m_2)}{d\Omega}$$
$$= \frac{2\pi C}{2J_0+1}[4\pi(2K_1+1)]^{1/2} \sum_{K_1} \mathcal{B}^{\rm ex}(0, K_1, K_1, 0, K_1, 0, 0, 0, K_1) Y_{K_1N_1}(\hat{p}_1). \qquad (32)$$

More simple expression can be obtained by coinciding the laboratory z axis with the direction of $\mathbf{p}_1$:

$$\sigma_{K_10}(\alpha_0 J_0 \to \alpha_1 J_1) = \frac{2\pi C}{2J_0+1} \sum_{K_1} (2K_1+1) \mathcal{B}^{\rm ex}(0, K_1, K_1, 0, K_1, 0, 0, 0, K_1). \qquad (33)$$

The alignment parameters obtains the following expression:

$$A_{K_1} = \frac{(2K_1+1)\mathcal{B}^{\rm ex}(0, K_1, K_1, 0, K_1, 0, 0, 0, K_1)}{\mathcal{B}^{\rm ex}(0, 0, 0, 0, 0, 0, 0, 0, 0)}. \qquad (34)$$

where $K_1 = 2, 4, ..., 2J_1$. In the case of $J_1 = 0$ and $J = 1/2$, the excited atoms can not be aligned because of $K_1 \leq 2$. For $J_1 = 1$, the alignment of excited atoms is described by the expression:

$$A_2 = \frac{5\mathcal{B}^{\rm ex}(0, 2, 2, 0, 2, 0, 0, 0, 2)}{\mathcal{B}^{\rm ex}(0, 0, 0, 0, 0, 0, 0, 0, 0)}. \qquad (35)$$

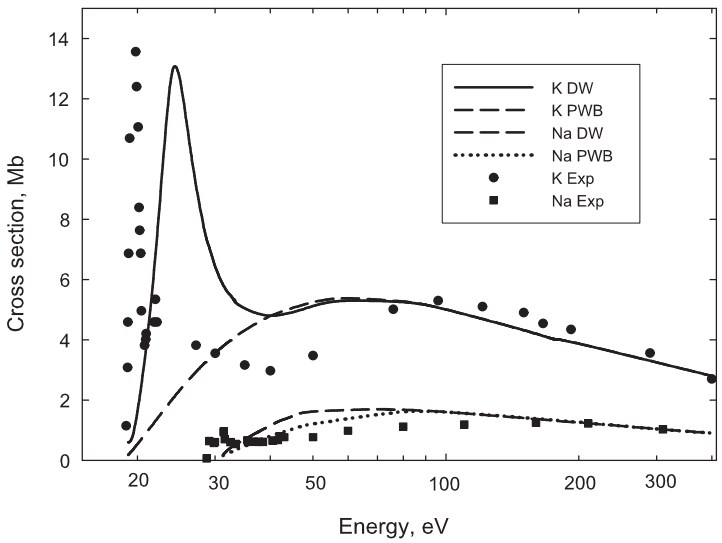

Figure 3 The comparison of calculated electron-impact excitation cross sections $2p^6 3s \rightarrow 2p^5 3s^2\ ^2P$ and $3p^6 4s \rightarrow 3p^5 4s^2\ ^2P_{3/2}$ with experimental data for Na [20] and K [21, 22].

4. Applications and discussion

The derived expressions for the total cross section (17), reduced matrix elements $\langle \alpha_1 J_1, \varepsilon_2 \lambda_2(j_2) J || H || \alpha_0 J_0, \varepsilon_1 \lambda_1(j_1) J \rangle$, the asymmetry parameter of the angular distribution of the scattered electrons β_K (20), the alignment parameters A (34) of unpolarized atoms excited in the case of unpolarized electrons as well as the degree of magnetic dichroism a (28) of the excitation of polarized atoms by unpolarized electrons are used in the creation of computer program in FORTRAN. The calculations of the total cross section and alignment parameter for the excitation the autoionizing states of $2p^5 3s^2\ ^2P_{3/2}$ for Na and $3p^5 4s^2\ ^2P_{3/2}$ for K are carried out as an example. The cross sections are displayed in figure 3, and the alignment parameters are shown in figure 4. The distorted wave (DW) with exchange approximation and multiconfiguration wave functions [19] are used. The calculations in plane wave Born (PWB) approximation were also performed in the present work. The correlation effects are important and decrease the values of the cross section about 7% for Na and 8% for K. It can be expected because the dominant expansions are 0.96 $2p^5 3s^2$+0.26 $2p^5 3p^2$ and 0.95 $3p^5 4s^2$+0.30 $3p^5 4p^2$ −0.09 $3p^5 4s(^1P)3d$−0.09 $3p^5 4s(^3P)3d$ for Na and K, respectively. In the case of Na, the cross sections for the term ^2P were calculated in order to make the comparison with experimental data [20]. The cross sections calculated in DW and PWB approximations are in close agreement with those obtained by Borovik *et al* [21] in the same approximations, therefore they are not presented in figure 3 for comparison.

The results from figure 3 show that the values of calculated cross sections merge with experimental data [20, 21, 22] for the incident electron energies about three times

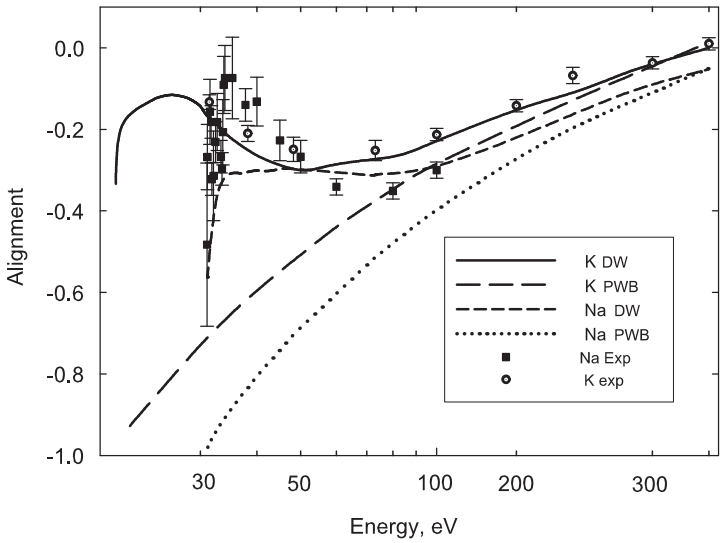

Figure 4 The alignment parameters of electron-impact excited state $2p^6 3s \rightarrow 2p^5 3s^2\ ^2P_{3/2}$ for Na and $3p^6 4s \rightarrow 3p^5 4s^2\ ^2P_{3/2}$ for K calculated in DW and PWB approximations. Experimental data are presented for Na [13] and K [23].

larger than excitation threshold both for Na and K. A sharp increase of the excitation cross section near threshold for K is caused by the exchange scattering as it disappears in the cross section calculated in DW without exchange.

The results of figure 4 show that calculated in DW approximation alignment parameters of the state $3p^5 4s^2\ ^2P_{3/2}$ in K excited by electron impact are in good agreement with experimentally determined [23] over a broad range of incident electron energies. This agreement can be explained that an important part of the excitation mechanisms cancels in the ratio of the excitation cross sections for different magnetic sublevels. The values of the alignment parameter for K of the present work are close to those obtained by Materstock *et al* [23] in DW approximation with exchange using some optical potential. For the excitation energies exceeding the threshold twice, the calculated alignment parameters for Na in the state $2p^5 3s^2\ ^2P_{3/2}$ are also in good agreement with experimental data [13] and values calculated by applying *R*-matrix approach [13]. Significant deviations of the alignment parameters calculated in the present work from those of experimental data and *R*-matrix calculations can be noticed close to the excitation threshold indicating the importance of the correlations in the continuum. For large excitation energies, the PWB approximation can be used to calculate the alignment parameters for Na and K atoms.

5. Concluding remarks

The general expression for the cross section describing the excitation of polarized atoms by polarized electrons as a multiple expansion over the multipoles of the states of all particles participating in the process both in the initial and final states was obtained for the first time. A simple way to derive expressions for special cases by using the general expression is described. In the case of the excitation of unpolarized atoms by unpolarized electrons, more simple expressions for the total cross section, parameters of the alignment of excited atoms and the asymmetry parameters of the angular distribution of the scattered electrons are obtained from the general expression. The derivation of the degree of magnetic dichroism as well as the parameters of the asymmetry of the angular distribution of scattered electrons in the case of the excitation of polarized atoms by unpolarized electrons are also demonstrated by using the general expression. The special expressions are implemented into computer code. The calculations of the total cross section and alignment parameter for the excitation the autoionizing states of $2p^5 3s^2\ ^2P_{3/2}$ for Na and $3p^5 4s^2\ ^2P_{3/2}$ for K are carried out as an example. The calculated in DW approximation alignment parameters of the state $3p^5 4s^2\ ^2P_{3/2}$ in K excited by electron impact are in good agreement with those experimentally determined over a broad range of incident electron energies. Significant deviations of the alignment parameters calculated in the present work from those of experimental data and *R*-matrix calculations noticed close to the excitation threshold indicate the importance of the correlations in the continuum.

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